

Solvable Model of a Mixture of Bose-Einstein Condensates

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Abstract

A mixture of two kinds of identical bosons held in a harmonic potential and interacting by harmonic particle-particle interactions is discussed. This is an exactly-solvable model of a mixture of two trapped Bose-Einstein condensates which allows us to examine analytically various properties. Generalizing the treatment in [Cohen and Lee, J. Math. Phys. **26**, 3105 (1985)], closed form expressions for the ground-state energy, wave-function, and lowest-order densities are obtained and analyzed for attractive and repulsive intra-species and inter-species particle-particle interactions. A particular mean-field solution of the corresponding Gross-Pitaevskii theory is also found analytically. This allows us to compare properties of the mixture at the exact, many-body and mean-field levels, both for finite systems and at the limit of an infinite number of particles. We hereby prove that the exact ground-state energy and lowest-order intra-species and inter-species densities converge at the infinite-particle limit (when the products of the number of particles times the intra-species and inter-species interaction strengths are held fixed) to the results of the Gross-Pitaevskii theory for the mixture. Finally and on the other end, the separability of the mixture's center-of-mass coordinate is used to show that the Gross-Pitaevskii theory for mixtures is unable to describe the variance of many-particle operators in the mixture, even in the infinite-particle limit. Our analytical results show that many-body correlations exist in a mixture of Bose-Einstein condensates made of any number of particles. Implications are briefly discussed.

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I. INTRODUCTION

Mixtures of Bose-Einstein condensates, following their first experimental realizations in ultra-cold atoms [1–4], have been immensely explored theoretically for their ground state and excitations, statics and out-of-equilibrium dynamics, at zero and finite temperatures, when miscible or immiscible, and in traps of various shapes and topologies, see, e.g., [5–52], representing in our viewing how fascinating and rich these quantum systems are. Methodologically, bosonic mixtures have been treated by a variety of many-body approaches and numerical tools, as well as within Gross-Pitaevskii, mean-field theory. Whereas the Gross-Pitaevskii theory is often employed, only the use of many-body theory can actually ensure when the mean-field theory provides an adequate description and when it is not. Obviously and quite generally, a many-body description is more demanding than a mean-field description. In this respect, having an exactly-solvable many-body model at hand is, of course, the ideal situation.

In this work we present such an exactly-solvable model of a mixture of two trapped Bose-Einstein condensates. Explicitly, we consider two kinds of identical bosons held in a harmonic potential and interacting by harmonic particle-particle interactions, or, briefly, the harmonic-interaction model (HIM) for bosonic mixtures. We emphasize that the HIM model for single-species bosons is well known and has provided ample many-body, exact results as well as means to benchmark numerical investigations [53–58]. Similarly, the HIM model for fermions has been employed, see, e.g., [54, 59, 60]. We would also like to mention the use of an analytical treatment based on coupled harmonic oscillators for vibrations [61], which are distinguishable degrees of freedom.

The mixture’s HIM model to be derived below allows us to examine analytically various properties, in particular the ground-state energy, wave-function, and lowest-order intra-species and inter-species densities, and how they depend on the number of particles and interactions in the mixture. A plethora of exact, many-body results is reported and analyzed.

In addition, we also find analytically the ground-state solution of the Gross-Pitaevskii theory for the mixture’s HIM. This enables us to compare properties of the mixture at the exact, many-body and mean-field levels, both for finite mixtures and in the limit of an infinite number of particles. The later topic, i.e., when the many-body and mean-field descriptions of a Bose-Einstein condensate coincide, is of much interest for single-species

bosons [62–67], but has yet to be addressed for mixtures. We hereby prove that the exact ground-state energy and lowest-order intra-species and inter-species densities converge at the infinite-particle limit to the results of the Gross-Pitaevskii theory for the mixture.

Last but not least, the separability of the mixture’s center-of-mass coordinate is used to show that the Gross-Pitaevskii theory for mixtures can deviate strongly when computing the variance of many-particle operators in the mixture, even in the infinite-particle limit. Unlike the variance of operators of a single particle, which is a basic notion in any quantum mechanics textbook [68], the variance of operators of many-particle systems is more involved [66, 67], also see [69] in this context. Our analytical results show that many-body correlations exist in a trapped mixture of Bose-Einstein condensates consisting of *any number of particles*.

II. THE HARMONIC-INTERACTION MODEL FOR MIXTURES

Consider a mixture of two kinds of identical bosons which we denote A and B . The bosons are trapped in a three-dimensional isotropic harmonic potential and interact between them via harmonic particle-particle interactions. We focus in this work on what might be considered the simplest case, the symmetric mixture. This is a mixture consisting of M bosons of type A and an equal number of M bosons of type B , all having the same mass (taken below to be 1) and trapped in the same harmonic potential (of frequency ω). The total number of particles is denoted by $N = 2M$. Furthermore, the two intra-species interactions are alike (denoted by λ_1). The inter-species interaction is denoted by λ_2 . Positive values of λ_1 and λ_2 mean attractive particle-particle interactions whereas negative values imply repulsive interactions. Of course, the intra-species interactions may be repulsive and the inter-species attractive, and vice versa.

The mixture’s Hamiltonian is then given by ($\hbar = 1$)

$$\begin{aligned} \hat{H}(\mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}_1, \dots, \mathbf{y}_M) = & \sum_{j=1}^M \left[\left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{x}_j^2} + \frac{1}{2} \omega^2 \mathbf{x}_j^2 \right) + \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{y}_j^2} + \frac{1}{2} \omega^2 \mathbf{y}_j^2 \right) \right] + \\ & + \lambda_1 \sum_{1 \leq j < k}^M [(\mathbf{x}_j - \mathbf{x}_k)^2 + (\mathbf{y}_j - \mathbf{y}_k)^2] + \lambda_2 \sum_{j=1}^M \sum_{k=1}^M (\mathbf{x}_j - \mathbf{y}_k)^2. \end{aligned} \quad (1)$$

Here, the coordinates \mathbf{x}_j denote bosons of type A and \mathbf{y}_k bosons of type B . We work in Cartesian coordinates where the vector $\mathbf{x} = (x_1, x_2, x_3)$ denotes an A particle’s position in three dimensions, and $\frac{1}{i} \frac{\partial}{\partial \mathbf{x}} = \frac{1}{i} \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right)$ its momentum. To avoid cumbersome

notation, we denote $\mathbf{x}^2 \equiv x_1^2 + x_2^2 + x_3^2$ and $\frac{\partial^2}{\partial \mathbf{x}^2} \equiv \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$. Analogous notation is employed for the vector \mathbf{y} of the B species bosons. In what follows and when needed, we use the vector \mathbf{r} to denote the position of a particle of either kind. Opening the braces of the particle-particle interaction terms and collecting the diagonal contributions together we have

$$\begin{aligned} \hat{H} = & \sum_{j=1}^M \left\{ -\frac{1}{2} \left(\frac{\partial^2}{\partial \mathbf{x}_j^2} + \frac{\partial^2}{\partial \mathbf{y}_j^2} \right) + \frac{1}{2} [\omega^2 + (N-2)\lambda_1 + N\lambda_2] (\mathbf{x}_j^2 + \mathbf{y}_j^2) \right\} - \\ & -2\lambda_1 \sum_{1 \leq j < k}^M (\mathbf{x}_j \cdot \mathbf{x}_k + \mathbf{y}_j \cdot \mathbf{y}_k) - 2\lambda_2 \sum_{j=1}^M \sum_{k=1}^M \mathbf{x}_j \cdot \mathbf{y}_k. \end{aligned} \quad (2)$$

As we shall see below, it is instrumental to combine the j th coordinate in the A and B species together.

To diagonalize the Hamiltonian (1) we build on the single-species HIM transformed coordinates [53] (here, for each of the A and B species) and make the following coordinate transformation

$$\begin{aligned} \mathbf{Q}_k &= \frac{1}{\sqrt{k(k+1)}} \sum_{j=1}^k (\mathbf{x}_{k+1} - \mathbf{x}_j), \quad 1 \leq k \leq M-1, \\ \mathbf{Q}_{M-1+k} &= \frac{1}{\sqrt{k(k+1)}} \sum_{j=1}^k (\mathbf{y}_{k+1} - \mathbf{y}_j), \quad 1 \leq k \leq M-1, \\ \mathbf{Q}_{N-1} &= \frac{1}{\sqrt{N}} \sum_{j=1}^M (\mathbf{x}_j - \mathbf{y}_j), \\ \mathbf{Q}_N &= \frac{1}{\sqrt{N}} \sum_{j=1}^M (\mathbf{x}_j + \mathbf{y}_j). \end{aligned} \quad (3)$$

The meaning of (3) is as follows: The first group of $M-1$ coordinates are relative coordinates of the A species; the second group of $M-1$ coordinates are relative coordinates of the B species; \mathbf{Q}_{N-1} can be seen as a relative coordinate between the center-of-mass of the A species and the center-of-mass of the B species; and, finally, \mathbf{Q}_N is (proportional to) the center-of-mass coordinate of all particles in the mixture. Further discussion of this coordinate transformation is given in the Appendix. With the coordinate transformation (3) the kinetic energy remains diagonal,

$$\sum_{j=1}^M \left(\frac{\partial^2}{\partial \mathbf{x}_j^2} + \frac{\partial^2}{\partial \mathbf{y}_j^2} \right) = \sum_{k=1}^N \frac{\partial^2}{\partial \mathbf{Q}_k^2}, \quad (4)$$

and the following quadratic relations hold

$$\begin{aligned}
\sum_{k=1}^{N-2} \mathbf{Q}_k^2 &= \left(1 - \frac{2}{N}\right) \sum_{j=1}^M (\mathbf{x}_j^2 + \mathbf{y}_j^2) - \frac{4}{N} \sum_{1 \leq j < k}^M (\mathbf{x}_j \cdot \mathbf{x}_k + \mathbf{y}_j \cdot \mathbf{y}_k), \\
\mathbf{Q}_{N-1}^2 &= \frac{1}{N} \left\{ \sum_{j=1}^M (\mathbf{x}_j^2 + \mathbf{y}_j^2) + 2 \left[\sum_{1 \leq j < k}^M (\mathbf{x}_j \cdot \mathbf{x}_k + \mathbf{y}_j \cdot \mathbf{y}_k) - \sum_{j=1}^M \sum_{k=1}^M \mathbf{x}_j \cdot \mathbf{y}_k \right] \right\}, \\
\mathbf{Q}_N^2 &= \frac{1}{N} \left\{ \sum_{j=1}^M (\mathbf{x}_j^2 + \mathbf{y}_j^2) + 2 \left[\sum_{1 \leq j < k}^M (\mathbf{x}_j \cdot \mathbf{x}_k + \mathbf{y}_j \cdot \mathbf{y}_k) + \sum_{j=1}^M \sum_{k=1}^M \mathbf{x}_j \cdot \mathbf{y}_k \right] \right\}. \tag{5}
\end{aligned}$$

Using (3), (4), and (5), the Hamiltonian (1) transforms to the diagonal form

$$\begin{aligned}
\hat{H}(\mathbf{Q}_1, \dots, \mathbf{Q}_N) &= \sum_{k=1}^{N-2} \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{Q}_k^2} + \frac{1}{2} \Omega_{rel}^2 \mathbf{Q}_k^2 \right) + \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{Q}_{N-1}^2} + \frac{1}{2} \Omega_{AB}^2 \mathbf{Q}_{N-1}^2 \right) + \\
&+ \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{Q}_N^2} + \frac{1}{2} \omega^2 \mathbf{Q}_N^2 \right). \tag{6}
\end{aligned}$$

The mixture's transformed Hamiltonian (6) is that of N uncoupled harmonic oscillators with the three frequencies

$$\Omega_{rel} = \sqrt{\omega^2 + N(\lambda_1 + \lambda_2)}, \quad \Omega_{AB} = \sqrt{\omega^2 + 2N\lambda_2}, \quad \omega. \tag{7}$$

The multiplicity of the frequencies is $N - 2$, 1, and 1, respectively.

Let us examine the frequencies (7) and their dependence on the particle-particle interactions more closely. The frequency of all intra-species relative coordinates $\mathbf{Q}_1, \dots, \mathbf{Q}_{2(M-1)}$, Ω_{rel} , depends on both the intra-species λ_1 and inter-species λ_2 interactions, yet only through their sum $\lambda_1 + \lambda_2$. The frequency Ω_{AB} of the intra-species relative coordinate \mathbf{Q}_{N-1} depends on λ_2 only. The frequency of the center-of-mass degree of freedom \mathbf{Q}_N , which is equal to the trap frequency ω , naturally does not depend on either. When $\lambda_1 = 0$, i.e., when the intra-species interactions vanish, we are still dealing with a mixture described by three frequencies, solely due to the inter-species interaction which couples all N particles together. On the other hand, when $\lambda_1 + \lambda_2 = 0$, we get $\Omega_{rel} = \omega$ and the mixture is now described by two frequencies only. We will analyze this case further below. When the intra- and inter-species interactions are equal, $\lambda_1 = \lambda_2$, the frequency of the relative coordinate between the center-of-masses of the A and B species degenerates to that of the other relative coordinates, i.e., $\Omega_{AB} = \Omega_{rel}$, and the standard, single-species HIM model of N bosons is recovered. Finally, in the limiting case when $\lambda_2 = 0$, we have $\Omega_{AB} = \omega$ and, as one would expect, we find two independent species each described by the HIM model for M bosons.

The frequencies (7) must be positive in order for a bound solution to exist. This dictates bounds on both the intra-species λ_1 and inter-species λ_2 interactions which are:

$$\begin{aligned}\Omega_{AB}^2 = \omega^2 + 2N\lambda_2 > 0 &\implies \lambda_2 > -\frac{\omega^2}{2N}, \\ \Omega_{rel}^2 = \omega^2 + N(\lambda_1 + \lambda_2) > 0 &\implies \lambda_1 > -\lambda_2 + \frac{\omega^2}{N}.\end{aligned}\quad (8)$$

The meaning of these bounds are as follows: The inter-species interaction λ_2 is bounded from below, irrespective of the intra-species interaction λ_1 , otherwise the mixture cannot be trapped in the harmonic potential. On the other hand, the intra-species interaction λ_1 is limited by the chosen inter-species interaction λ_2 .

We can now proceed and prescribe the normalized ground-state wave-function

$$\Psi(\mathbf{Q}_1, \dots, \mathbf{Q}_N) = \left(\frac{\Omega_{rel}}{\pi}\right)^{\frac{3(N-2)}{4}} \left(\frac{\Omega_{AB}}{\pi}\right)^{\frac{3}{4}} \left(\frac{\omega}{\pi}\right)^{\frac{3}{4}} e^{-\frac{1}{2}(\Omega_{rel} \sum_{k=1}^{N-2} \mathbf{Q}_k^2 + \Omega_{AB} \mathbf{Q}_{N-1}^2 + \omega \mathbf{Q}_N^2)}, \quad (9)$$

along with the ground-state eigen-energy

$$E = \frac{3}{2} [(N-2)\Omega_{rel} + \Omega_{AB} + \omega] = \frac{3}{2} \left[(N-2)\sqrt{\omega^2 + N(\lambda_1 + \lambda_2)} + \sqrt{\omega^2 + 2N\lambda_2} + \omega \right]. \quad (10)$$

To express the wave-function with respect to the original spatial coordinates we use the relations (5) and find

$$\begin{aligned}\Psi(\mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}_1, \dots, \mathbf{y}_M) &= \left(\frac{\Omega_{rel}}{\pi}\right)^{\frac{3(N-2)}{4}} \left(\frac{\Omega_{AB}}{\pi}\right)^{\frac{3}{4}} \left(\frac{\omega}{\pi}\right)^{\frac{3}{4}} \times \\ &\times e^{-\frac{\alpha}{2} \sum_{j=1}^M \mathbf{x}_j^2 - \beta \sum_{1 \leq j < k}^M \mathbf{x}_j \cdot \mathbf{x}_k} \times e^{-\frac{\alpha}{2} \sum_{j=1}^M \mathbf{y}_j^2 - \beta \sum_{1 \leq j < k}^M \mathbf{y}_j \cdot \mathbf{y}_k} \times e^{+\gamma \sum_{j=1}^M \sum_{k=1}^M \mathbf{x}_j \cdot \mathbf{y}_k},\end{aligned}\quad (11)$$

where

$$\alpha = \Omega_{rel} \left(1 - \frac{2}{N}\right) + (\Omega_{AB} + \omega) \frac{1}{N} = \Omega_{rel} + \beta, \quad \beta = \frac{1}{N}(-2\Omega_{rel} + \Omega_{AB} + \omega), \quad \gamma = \frac{1}{N}(\Omega_{AB} - \omega). \quad (12)$$

The mixture's ground-state wave-function (11) is seen to be comprised of a product of an A part, an equivalent B part, and a coupling AB part.

III. PROPERTIES AND ANALYSIS

The HIM model for a mixture of two Bose-Einstein condensates presented above admits a wealth of properties that can all be studied analytically. We present in this section a

rather detailed account of the ground-state energy, intra- and inter-species densities, a mean-field solution, and the variance of center-of-mass operators in the mixture. Side by side the plethora of closed-form expressions and results, a guiding line of our exploration are properties of finite mixtures as well as at the infinite-particle limit (to be defined precisely below), and how the many-body and mean-field solutions are related to each other.

A. Ground-state energy

It is instructive and interesting to analyze the ground-state energy (10) in several cases. As mentioned above, for $\lambda_1 = \lambda_2$ we recover the ground-state energy of the single-species HIM model [53]. Keeping λ_1 and λ_2 fixed and increasing the number of particles N the energy to leading order in N scales like $N^{\frac{3}{2}}$, i.e. adding more particles increases further the mixture's energy. This situation applies as long as the bounds (8) are not reached, that is when the mixture is predominantly attractive, $\lambda_1 + \lambda_2 > 0$ and $\lambda_2 > 0$.

An interesting situation occurs for $\lambda_1 + \lambda_2 = 0$, i.e., when the intra- and inter-species interactions are exactly opposite in sign. In this case, as we touched upon above, Ω_{rel} degenerates to ω , and the energy (10) reduces to

$$E|_{\lambda_1+\lambda_2=0} = \frac{3}{2} \left[(N-1)\omega + \sqrt{\omega^2 + 2N\lambda_2} \right] \quad (13)$$

and seen to depend only on the inter-species interaction λ_2 . Now, the ground-state energy (13) is linear to leading order in the number of particles N .

Using the bounds for λ_1 and λ_2 in (8), we obtain that the mixture's energy is bound from below by $E > \frac{3}{2}\omega$, which is obtained for $\Omega_{rel} \rightarrow 0^+$ and $\Omega_{AB} \rightarrow 0^+$. This means that all relative degrees of freedom are marginally bound, and essentially only the center-of-mass degree of freedom is bound in the harmonic trap.

We now move to analyze the mixture's energy in the so-called infinite-particle limit. To this end, we introduce the intra-species $\Lambda_1 = \lambda_1(M-1)$ and inter-species $\Lambda_2 = \lambda_2 M$ interaction parameters. In the infinite-particle limit the interaction parameters Λ_1 and Λ_2 are kept fixed, while the number of particles is increased. Hence, the interaction strengths λ_1 and λ_2 diminish accordingly. The two interaction parameters Λ_1 and Λ_2 appear naturally in the mean-field treatment discussed below, and would facilitate the comparison between the exact, many-body and mean-field solutions of the mixture.

Keeping Λ_1 and Λ_2 constant, the energy per particle in the limit of an infinite number of particles reads

$$\lim_{N \rightarrow \infty} \frac{E}{N} = \frac{3}{2} \sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}. \quad (14)$$

We see that the limit of the energy per particle depends on the sum of intra- and inter-species interaction parameters $\Lambda_1 + \Lambda_2$ only. Finally, in the particular case when the interaction parameters are fixed and opposite in sign, i.e., $\Lambda_1 + \Lambda_2 = 0$, we find in the infinite-particle limit

$$\lim_{N \rightarrow \infty} \frac{E|_{\Lambda_1 + \Lambda_2 = 0}}{N} = \frac{3}{2} \omega. \quad (15)$$

The meaning of (15) is that the energy per particle of the interacting system becomes that of the non-interacting system; A situation that cannot occur in the single-species system. Here, the intra- and inter-species interaction parameters ‘cancel’ each other in the infinite-particle limit, at least as far as the energy per particle is concerned. We will return to this peculiar situation below when analyzing the density and mean-field solution of the mixture.

B. Intra- and inter-species densities

We start from the N -particle density of the mixture

$$|\Psi(\mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}_1, \dots, \mathbf{y}_M)|^2 = \left(\frac{\Omega_{rel}}{\pi} \right)^{\frac{3(N-2)}{2}} \left(\frac{\Omega_{AB}}{\pi} \right)^{\frac{3}{2}} \left(\frac{\omega}{\pi} \right)^{\frac{3}{2}} \times \quad (16)$$

$$\times e^{-\alpha \sum_{j=1}^M \mathbf{x}_j^2 - 2\beta \sum_{1 \leq j < k}^M \mathbf{x}_j \cdot \mathbf{x}_k} \times e^{-\alpha \sum_{j=1}^M \mathbf{y}_j^2 - 2\beta \sum_{1 \leq j < k}^M \mathbf{y}_j \cdot \mathbf{y}_k} \times e^{+2\gamma \sum_{j=1}^M \sum_{k=1}^M \mathbf{x}_j \cdot \mathbf{y}_k},$$

which for convenience is here normalized to unity. Let the AB two-body density be

$$\rho_{AB}(\mathbf{x}, \mathbf{y}) = M^2 \int d\mathbf{x}_2 \cdots d\mathbf{x}_M d\mathbf{y}_2 \cdots d\mathbf{y}_M |\Psi(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_M, \mathbf{y}, \mathbf{y}_2, \dots, \mathbf{y}_M)|^2. \quad (17)$$

It is the lowest-order inter-species density of the mixture. Then, the intra-species one-body densities are given by

$$\rho_A(\mathbf{x}) = \frac{1}{M} \int d\mathbf{y} \rho_{AB}(\mathbf{x}, \mathbf{y}) \equiv \frac{1}{M} \int d\mathbf{x} \rho_{AB}(\mathbf{x}, \mathbf{y}) = \rho_B(\mathbf{y}), \quad (18)$$

and normalized to the number of bosons of each kind, M .

To obtain the lowest-order intra- and inter-species densities (18) and (17), respectively, we need to perform *multiple* integrations of the N -particle density (16). Moreover, the later contains a coupling AB part because of the inter-species interaction, also see below

(11). Thus, without an appropriate construction, the task becomes quickly impractical with increasing N . Fortunately, we are able to generalize the very useful recurrence integration construction for the densities of the single-species HIM put forward in [53] to the mixture's HIM model (1).

To integrate the N -particle density we begin by introducing the auxiliary function

$$\begin{aligned}
F_M(\mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}_1, \dots, \mathbf{y}_M; \alpha, \beta, C_M, D_M) &= \\
&= e^{-\alpha \sum_{j=1}^M (\mathbf{x}_j^2 + \mathbf{y}_j^2) - 2\beta \sum_{1 \leq j < k}^M (\mathbf{x}_j \cdot \mathbf{x}_k + \mathbf{y}_j \cdot \mathbf{y}_k) - C_M (\mathbf{X}_M + \mathbf{Y}_M)^2 + 2D_M \mathbf{X}_M \cdot \mathbf{Y}_M} = \\
&= e^{-\alpha \sum_{j=1}^M (\mathbf{x}_j^2 + \mathbf{y}_j^2) - 2\beta \sum_{1 \leq j < k}^M (\mathbf{x}_j \cdot \mathbf{y}_k + \mathbf{y}_j \cdot \mathbf{y}_k) - C_M (\mathbf{X}_M^2 + \mathbf{Y}_M^2) + 2(D_M - C_M) \mathbf{X}_M \cdot \mathbf{Y}_M}, \tag{19}
\end{aligned}$$

where α , β , and γ are given in (12),

$$\mathbf{X}_M = \sum_{j=1}^M \mathbf{x}_j, \quad \mathbf{Y}_M = \sum_{j=1}^M \mathbf{y}_j, \tag{20}$$

are vectors, and C_M and D_M are constants to play a further role below. We note that if one were to equate the N -body density (16) and the auxiliary function F_M then this would imply that $C_M = 0$ and $D_M = \gamma$. Finally, we note that the following relations

$$\begin{aligned}
\mathbf{X}_M^2 + \mathbf{Y}_M^2 &= \mathbf{X}_{M-1}^2 + \mathbf{Y}_{M-1}^2 + [\mathbf{x}_M^2 + \mathbf{y}_M^2 + 2(\mathbf{x}_M \cdot \mathbf{X}_{M-1} + \mathbf{y}_M \cdot \mathbf{X}_{M-1})], \\
\mathbf{X}_M \cdot \mathbf{Y}_M &= \mathbf{X}_{M-1} \cdot \mathbf{Y}_{M-1} + [\mathbf{x}_M \cdot \mathbf{Y}_{M-1} + \mathbf{y}_M \cdot \mathbf{X}_{M-1} + \mathbf{x}_M \cdot \mathbf{y}_M], \tag{21}
\end{aligned}$$

hold between the vectors introduced in (20) and the pair of variables \mathbf{x}_M and \mathbf{y}_M .

The key point is to perform the integrations in pairs reducing thereby the order of the auxiliary function F_M . The basic ingredient is the double-Gaussian integral over \mathbf{x}_j and \mathbf{y}_j

$$\begin{aligned}
&\int d\mathbf{x}_j d\mathbf{y}_j e^{-a(\mathbf{x}_j^2 + \mathbf{y}_j^2) - 2[\mathbf{x}_j \cdot (b\mathbf{X}_{j-1} + b'\mathbf{Y}_{j-1}) + \mathbf{y}_j \cdot (b\mathbf{Y}_{j-1} + b'\mathbf{X}_{j-1})] + 2c\mathbf{x}_j \cdot \mathbf{y}_j} = \\
&= \frac{\pi^3}{(a^2 - c^2)^{\frac{3}{2}}} e^{+p(\mathbf{X}_{j-1}^2 + \mathbf{Y}_{j-1}^2) + 2q\mathbf{X}_{j-1} \cdot \mathbf{Y}_{j-1}}, \tag{22}
\end{aligned}$$

where a , b , b' , c , p , and q are scalars connected by the relations

$$p = \frac{a(b^2 + b'^2) + 2bb'c}{a^2 - c^2}, \quad q = \frac{c(b^2 + b'^2) + 2abb'}{a^2 - c^2}, \quad (a \mp c)(p \pm q) = (b \pm b')^2. \tag{23}$$

Furthermore, to perform multiple double-integration steps like (22), we seek for a recurrence

relation and thus write

$$\begin{aligned}
& \int d\mathbf{x}_M d\mathbf{y}_M F_M = \\
& = e^{-\alpha \sum_{j=1}^{M-1} (\mathbf{x}_j^2 + \mathbf{y}_j^2) - 2\beta \sum_{1 \leq j < k} (\mathbf{x}_j \cdot \mathbf{x}_k + \mathbf{y}_j \cdot \mathbf{y}_k) - C_M (\mathbf{X}_{M-1}^2 + \mathbf{Y}_{M-1}^2) + 2(D_M - C_M) \mathbf{X}_{M-1} \cdot \mathbf{Y}_{M-1}} \times \\
& \int d\mathbf{x}_M d\mathbf{y}_M e^{-(\alpha + C_M)(\mathbf{x}_M^2 + \mathbf{y}_M^2)} \times \\
& e^{-2\{\mathbf{x}_M \cdot [(\beta + C_M) \mathbf{X}_{M-1} - (D_M - C_M) \mathbf{Y}_{M-1}] + 2\{\mathbf{y}_M \cdot [(\beta + C_M) \mathbf{Y}_{M-1} - (D_M - C_M) \mathbf{X}_{M-1}]\} + 2(D_M - C_M) \mathbf{x}_M \cdot \mathbf{y}_M} = \\
& = \frac{\pi^3}{[(\alpha + D_M)(\alpha + \tilde{C}_M)]^{\frac{3}{2}}} F_{M-1}(\mathbf{x}_1, \dots, \mathbf{x}_{M-1}, \mathbf{y}_1, \dots, \mathbf{y}_{M-1}; \alpha, \beta, C_{M-1}, D_{M-1}). \quad (24)
\end{aligned}$$

The equality (24) relates the auxiliary function F_M with $2M$ coordinates and constants C_M and D_M to the function F_{M-1} of the same functional form, with $2(M-1)$ coordinates and corresponding constants C_{M-1} and D_{M-1} . To simplify the relation between the constants in F_M and F_{M-1} , it is useful to take appropriate linear combinations. The final result reads

$$\begin{aligned}
\tilde{C}_{M-1} &= \tilde{C}_M - \frac{(\beta + \tilde{C}_M)^2}{\alpha + \tilde{C}_M}, & \tilde{C}_M &= (2C_M - D_M) = -\gamma, \\
D_{M-1} &= D_M - \frac{(\beta + D_M)^2}{\alpha + D_M}, & D_M &= \gamma,
\end{aligned} \quad (25)$$

where the values of \tilde{C}_M and D_M are obtained when we equate the auxiliary function F_M and the N -body density (16).

We can now write the recurrence relation connecting the function F_j with $2j$ variables and constants C_j and D_j to the function F_{j-1} with $2(j-1)$ variables and constants C_{j-1} and D_{j-1} . The equality looks like (24) and need not be pasted here. What is important is the recurrence relation between the corresponding constants which is given by

$$\begin{aligned}
\tilde{C}_{j-1} &= \tilde{C}_j - \frac{(\beta + \tilde{C}_j)^2}{\alpha + \tilde{C}_j}, & \tilde{C}_j &= (2C_j - D_j), \\
D_{j-1} &= D_j - \frac{(\beta + D_j)^2}{\alpha + D_j}.
\end{aligned} \quad (26)$$

In turn, the recursion ends with the ‘lowest-order’ auxiliary function

$$F_1(\mathbf{x}_1, \mathbf{y}_1; \alpha, \beta, C_1, D_1) = e^{-(\alpha + C_1)(\mathbf{x}_1^2 + \mathbf{y}_1^2) + 2(D_1 - C_1) \mathbf{x}_1 \cdot \mathbf{y}_1}. \quad (27)$$

As we shall see, the constants C_1 and D_1 are required to evaluate the intra- and inter-species densities of the mixture (18) and (17).

Interestingly and importantly, the recurrence relations (26) for the parameters \tilde{C}_j and D_j appearing in the double-Gaussian integrations of the mixture’s auxiliary function have

exactly the same structure as the recurrence relation emerging in the single-Gaussian integrations of the HIM system [53]. Thus, we use this result directly and write for the final result of the respective solutions

$$\begin{aligned}\tilde{C}_j &= -\alpha + \frac{(\alpha - \beta)(1 + j\eta_-)}{1 + (j + 1)\eta_-}, & D_j &= -\alpha + \frac{(\alpha - \beta)(1 + j\eta_+)}{1 + (j + 1)\eta_+}, \\ \eta_{\pm} &= \frac{(\alpha - \beta) - (\alpha \pm \gamma)}{(M + 1)(\alpha \pm \gamma) - M(\alpha - \beta)},\end{aligned}\quad (28)$$

where the initial conditions in (25) have been used [70].

We can now proceed to express explicitly the intra- and inter-species lowest-order densities. Because the auxiliary function F_M , together with the initial conditions $\tilde{C}_M = -\gamma$ and $D_M = \gamma$, is proportional to the N -particle density (16), the function F_1 is proportional to the intra-species two-body density (17). Thus we readily have

$$\begin{aligned}\rho_{AB}(\mathbf{x}, \mathbf{y}) &= M^2 \left[\frac{(\alpha + C_1)^2 - (D_1 - C_1)^2}{\pi^2} \right]^{\frac{3}{2}} e^{-(\alpha + C_1)(\mathbf{x}^2 + \mathbf{y}^2) + 2(D_1 - C_1)\mathbf{x} \cdot \mathbf{y}}, \\ &= M^2 \left[\frac{(\alpha + C_1)^2 - (D_1 - C_1)^2}{\pi^2} \right]^{\frac{3}{2}} e^{-\frac{1}{2}[(\alpha + C_1) + (D_1 - C_1)](\mathbf{x} - \mathbf{y})^2} e^{-\frac{1}{2}[(\alpha + C_1) - (D_1 - C_1)](\mathbf{x} + \mathbf{y})^2},\end{aligned}\quad (29)$$

for the two-body density and, upon one additional integration,

$$\begin{aligned}\rho_A(\mathbf{x}) &= M \left[\frac{(\alpha + D_1)(\alpha + \tilde{C}_1)}{\pi(\alpha + C_1)} \right]^{\frac{3}{2}} e^{-\frac{(\alpha + D_1)(\alpha + \tilde{C}_1)}{(\alpha + C_1)}\mathbf{x}^2}, \\ \rho_B(\mathbf{y}) &= M \left[\frac{(\alpha + D_1)(\alpha + \tilde{C}_1)}{\pi(\alpha + C_1)} \right]^{\frac{3}{2}} e^{-\frac{(\alpha + D_1)(\alpha + \tilde{C}_1)}{(\alpha + C_1)}\mathbf{y}^2},\end{aligned}\quad (30)$$

for the one-body densities. We see that the two-body density can be viewed as an ellipsoid in the \mathbf{x} - \mathbf{y} coordinates, see the second line of (29), whereas the one-body densities are isotropic Gaussians in \mathbf{x} and \mathbf{y} coordinates.

To complete the computation of the densities we are left to determine \tilde{C}_1 and D_1 as a function of the mixture's frequencies Ω_{rel} , Ω_{AB} , and ω and the number of particles in each species M . Using (12) we find

$$\begin{aligned}\alpha - \beta &= \Omega_{rel}, & \alpha + \gamma &= \frac{(M - 1)\Omega_{rel} + \Omega_{AB}}{M}, & \alpha - \gamma &= \frac{(M - 1)\Omega_{rel} + \omega}{M} & \implies \\ \eta_+ &= \frac{\Omega_{rel} - \Omega_{AB}}{(M + 1)\Omega_{AB} - \Omega_{rel}}, & \eta_- &= \frac{\Omega_{rel} - \omega}{(M + 1)\omega - \Omega_{rel}}.\end{aligned}\quad (31)$$

From which we obtain the ingredients

$$\begin{aligned}
\alpha + \tilde{C}_1 &= \Omega_{rel} \frac{M\omega}{(M-1)\omega + \Omega_{rel}}, \\
\alpha + D_1 &= \Omega_{rel} \frac{M\Omega_{AB}}{(M-1)\Omega_{AB} + \Omega_{rel}}, \\
\alpha + C_1 &= \frac{(\alpha + \tilde{C}_1) + (\alpha + D_1)}{2} = \Omega_{rel} \frac{M[2(M-1)\omega\Omega_{AB} + (\omega + \Omega_{AB})\Omega_{rel}]}{2[(M-1)\omega + \Omega_{rel}][(M-1)\Omega_{AB} + \Omega_{rel}]},
\end{aligned} \tag{32}$$

and combinations thereof

$$\begin{aligned}
2(D_1 - C_1) &= (\alpha + D_1) - (\alpha + \tilde{C}_1) = \frac{M\Omega_{rel}^2(\Omega_{AB} - \omega)}{[(M-1)\omega + \Omega_{rel}][(M-1)\Omega_{AB} + \Omega_{rel}]}, \\
(\alpha + C_1)^2 - (D_1 - C_1)^2 &= (\alpha + D_1)(\alpha + \tilde{C}_1) = \Omega_{rel}^2 \frac{M^2\omega\Omega_{AB}}{[(M-1)\omega + \Omega_{rel}][(M-1)\Omega_{AB} + \Omega_{rel}]}, \\
\frac{(\alpha + D_1)(\alpha + \tilde{C}_1)}{(\alpha + C_1)} &= \frac{2}{\frac{1}{\alpha + D_1} + \frac{1}{\alpha + \tilde{C}_1}} = \Omega_{rel} \frac{2M\omega\Omega_{AB}}{2(M-1)\omega\Omega_{AB} + \Omega_{rel}(\omega + \Omega_{AB})}
\end{aligned} \tag{33}$$

entering the expressions (29) and (30). We have now computed explicitly and analytically the lowest-order densities of the mixture.

With analytical expressions for the densities one can examine various situations. We wish to elaborate on two. The two-body density couples the A and B species as soon as the inter-species interaction, λ_2 , is present, see (29). This is because $\lambda_2 \neq 0$ leads to $\Omega_{AB} \neq \omega$, see (7), which implies $(D_1 - C_1) \neq 0$, see the first line of (33). Furthermore, from the aspect ratio of the ellipsoid in the \mathbf{x} - \mathbf{y} coordinates, $(D_1 - C_1) > 0$ means that distinct particles tend to be together, i.e., inter-species attraction, whereas $(D_1 - C_1) < 0$ means that distinct particles tend to be apart from each other, i.e., inter-species repulsion. This is compatible with (33) which shows that $(D_1 - C_1)$ is positive (negative) when Ω_{AB} is bigger (smaller) than ω , i.e., when λ_2 is positive (negative). To remind, $\lambda_2 > 0$ signifies inter-species attraction and $\lambda_2 < 0$ repulsion.

The second issue we would like to discuss is the so-called infinite-particle limit. As mentioned in Sec. I, this question has drawn much attention for single-species Bose-Einstein condensates. With the help of the present analytical many-body results, and with the mean-field solution of the subsequent section, we can, to the best of our knowledge for the first time, give some concrete answers on what happens in the infinite-particle limit in a mixture. Thus, holding the intra- and inter-species interaction parameters Λ_1 and Λ_2 fixed, we have for the mixture's frequencies in the infinite-particle limit $\lim_{M \rightarrow \infty} \Omega_{rel} = \sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}$

and $\lim_{M \rightarrow \infty} \Omega_{AB} = \sqrt{\omega^2 + 4\Lambda_2}$. Now, the ingredients (32) entering the densities satisfy in the limit of an infinite number of particles $\lim_{M \rightarrow \infty}(\alpha + C_1) = \lim_{M \rightarrow \infty}(\alpha + D_1) = \lim_{M \rightarrow \infty}(\alpha + \tilde{C}_1) = \sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}$, and similarly in (33). Consequently, in the infinite-particle limit the expressions for the densities, see (18) and (17), depend on the interaction parameters only and simplify

$$\begin{aligned} \lim_{M \rightarrow \infty} \frac{\rho_A(\mathbf{x})}{M} &= \left(\frac{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}{\pi} \right)^{\frac{3}{2}} e^{-\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}\mathbf{x}^2}, \\ \lim_{M \rightarrow \infty} \frac{\rho_B(\mathbf{y})}{M} &= \left(\frac{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}{\pi} \right)^{\frac{3}{2}} e^{-\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}\mathbf{y}^2}, \end{aligned} \quad (34)$$

and

$$\lim_{M \rightarrow \infty} \frac{\rho_{AB}(\mathbf{x}, \mathbf{y})}{M^2} = \left(\frac{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}{\pi} \right)^3 e^{-\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}(\mathbf{x}^2 + \mathbf{y}^2)}. \quad (35)$$

In particular, because $\lim_{M \rightarrow \infty}(D_1 - C_1) = 0$ the inter-species two-body density is seen to factorize to a product of two one-body densities, independent of the magnitude of the inter-species interaction parameter Λ_2 . We would come back to this point in the following section, when the mean-field solution of the mixture's HIM model is to be derived and analyzed.

C. Mean-field (Gross-Pitaevskii) solution

At the other end of the exact, many-body solution of the mixture's HIM model lies the Gross-Pitaevskii, mean-field solution. In the mean-field theory the many-particle wavefunction is approximated as a product state, where all the bosons of the A species lies in the one and the same orbital, and all the bosons of the B species similarly lie in one orbital which is generally different than the A species one. In our case of a symmetric mixture (1), excluding a solution where demixing of the two species occurs in the ground state, the mean-field ansatz for the mixture is the product wave-function where, due to symmetry between the A and B species, each of the species occupies the same spatial function

$$\Phi^{GP}(\mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}_1, \dots, \mathbf{y}_M) = \prod_{j=1}^M \phi(\mathbf{x}_j) \prod_{k=1}^M \phi(\mathbf{y}_k). \quad (36)$$

The Gross-Pitaevskii energy functional of the mixture thus simplifies and reads

$$\begin{aligned}
\varepsilon^{GP} &= \frac{1}{2} \left[\int d\mathbf{x} \phi^*(\mathbf{x}) \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{x}^2} + \frac{1}{2} \omega^2 \mathbf{x}^2 \right) \phi(\mathbf{x}) + \frac{\Lambda_1}{2} \int d\mathbf{x} d\mathbf{x}' |\phi(\mathbf{x})|^2 |\phi(\mathbf{x}')|^2 (\mathbf{x} - \mathbf{x}')^2 + \right. \\
&+ \int d\mathbf{y} \phi^*(\mathbf{y}) \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{y}^2} + \frac{1}{2} \omega^2 \mathbf{y}^2 \right) \phi(\mathbf{y}) + \frac{\Lambda_2}{2} \int d\mathbf{y} d\mathbf{y}' |\phi(\mathbf{y})|^2 |\phi(\mathbf{y}')|^2 (\mathbf{y} - \mathbf{y}')^2 \left. \right] + \\
&+ \frac{\Lambda_2}{2} \int d\mathbf{x} d\mathbf{y} |\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2 (\mathbf{x} - \mathbf{y})^2 = \\
&= \int d\mathbf{r} \phi^*(\mathbf{r}) \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{1}{2} \omega^2 \mathbf{r}^2 \right) \phi(\mathbf{r}) + \frac{1}{2} (\Lambda_1 + \Lambda_2) \int d\mathbf{r} d\mathbf{r}' |\phi(\mathbf{r})|^2 |\phi(\mathbf{r}')|^2 (\mathbf{r} - \mathbf{r}')^2, \quad (37)
\end{aligned}$$

where \mathbf{r} represents the coordinate of any of the particles. To remind, ε^{GP} is the total mean-field energy of the mixture divided by the number of particle $N = 2M$. Consequently and side by side, the two coupled Gross-Pitaevskii equations of the mixture degenerate to one

$$\left\{ -\frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{1}{2} \omega^2 \mathbf{r}^2 + (\Lambda_1 + \Lambda_2) \int d\mathbf{r}' |\phi(\mathbf{r}')|^2 (\mathbf{r} - \mathbf{r}')^2 \right\} \phi(\mathbf{r}) = \mu \phi(\mathbf{r}), \quad (38)$$

where μ is the chemical potential of each species. The solution of (38) follows exactly the same way as for the HIM problem [53], and is now briefly followed for completeness.

Expanding the interaction term in (38) we find

$$\left\{ -\frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{1}{2} [\omega^2 + 2(\Lambda_1 + \Lambda_2)] \mathbf{r}^2 \right\} \phi(\mathbf{r}) = \left[\mu - (\Lambda_1 + \Lambda_2) \int d\mathbf{r}' |\phi(\mathbf{r}')|^2 \mathbf{r}'^2 \right] \phi(\mathbf{r}). \quad (39)$$

The solution of (39) is the Gaussian function.

$$\begin{aligned}
\phi(\mathbf{r}) &= \left(\frac{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}{\pi} \right)^{\frac{3}{4}} e^{-\frac{1}{2} \sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)} \mathbf{r}^2} = \\
&= \left(\frac{\sqrt{\Omega_{rel}^2 - 2\lambda_1}}{\pi} \right)^{\frac{3}{4}} e^{-\frac{1}{2} \sqrt{\Omega_{rel}^2 - 2\lambda_1} \mathbf{r}^2}. \quad (40)
\end{aligned}$$

Since the orbital (40) is an even function, there is no linear in \mathbf{r} term in (39). We can now evaluate the integral $\int d\mathbf{r}' |\phi(\mathbf{r}')|^2 \mathbf{r}'^2 = \frac{3}{2\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}$ in (39) and determine the chemical potential

$$\mu = \frac{3}{2} \sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)} + \frac{3}{4} \frac{\Lambda_1 + \Lambda_2}{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}} = \frac{3}{4} \frac{2\omega^2 + 3(\Lambda_1 + \Lambda_2)}{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}. \quad (41)$$

Indeed, for $\lambda_1 = \lambda_2$ the single-species HIM chemical potential [53] is found. With this, the mean-field energy is given by

$$\begin{aligned}
\varepsilon^{GP} &= \left\{ \mu - \frac{1}{2} (\Lambda_1 + \Lambda_2) \int d\mathbf{r} d\mathbf{r}' |\phi(\mathbf{r})|^2 |\phi(\mathbf{r}')|^2 (\mathbf{r} - \mathbf{r}')^2 \right\} = \\
&= \frac{3}{2} \sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)} = \frac{3}{2} \sqrt{\Omega_{rel}^2 - 2\lambda_1}, \quad (42)
\end{aligned}$$

where $\int d\mathbf{r}d\mathbf{r}'|\phi(\mathbf{r})|^2|\phi(\mathbf{r}')|^2(\mathbf{r}-\mathbf{r}')^2 = \frac{3}{\sqrt{\omega^2+2(\Lambda_1+\Lambda_2)}}$ is used. In the specific case where $\Lambda_1 + \Lambda_2 = 0$, the mean-field energy becomes that of the non-interacting system. This reminds the properties of the many-body energy discussed above, see (13) and (15) and associated text.

We can now compare the exact, many-body energy E and the mean-field energy per particle ε^{GP} . Of course, the many-body energy is always lower, for repulsive as well as for attractive particle-particle interactions, than the mean-field energy because of the variational principle. In the infinite-particle limit we find when Λ_1 and Λ_2 are held constant that

$$\lim_{N \rightarrow \infty} \frac{E}{N} = \varepsilon^{GP}, \quad (43)$$

which establishes the connection between the exact energy and mean-field (Gross-Pitaevskii) energy per particle in this limit for the mixture.

We now discuss the one-body density. From (40) we have

$$\begin{aligned} \rho^{GP}(\mathbf{r}) &= |\phi^{GP}(\mathbf{r})|^2 = \left(\frac{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}{\pi} \right)^{\frac{3}{2}} e^{-\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}\mathbf{r}^2} = \\ &= \left(\frac{\sqrt{\Omega_{rel}^2 - 2\lambda_1}}{\pi} \right)^{\frac{3}{2}} e^{-\sqrt{\Omega_{rel}^2 - 2\lambda_1}\mathbf{r}^2}. \end{aligned} \quad (44)$$

From the mean-field solution we see that the density narrows for overall attractive interactions and broadens for repulsive ones. To be more precise, the density narrows for $\Lambda_1 + \Lambda_2 > 0$ and broadens for $\Lambda_1 + \Lambda_2 < 0$. Within the mean-field theory this is the manifestation of the self-consistency used to solve the non-linear Schrödinger (Gross-Pitaevskii) equation and find the orbital (40). Furthermore, from (44) and using (36) we can write for the lowest-order densities of the mixture within the mean-field theory, $\rho_A^{GP}(\mathbf{x}) = M\rho^{GP}(\mathbf{x})$, $\rho_B^{GP}(\mathbf{y}) = M\rho^{GP}(\mathbf{y})$, and $\rho_{AB}^{GP}(\mathbf{x}, \mathbf{y}) = M^2\rho^{GP}(\mathbf{x})\rho^{GP}(\mathbf{y})$. As expected, for mixtures with a finite number of particles, the mean-field densities differ from their many-body counterparts (30) and (29). For instance, in contrast to the two-body inter-species density $\rho_{AB}(\mathbf{x}, \mathbf{y})$, the mean-field density $\rho_{AB}^{GP}(\mathbf{x}, \mathbf{y})$ is always factorized to a product of two one-body densities. Finally, in the limit of an infinite number of particles the many-body (35) and (34) and the Gross-Pitaevskii densities coincide in the sense that what one might have suspected holds true, namely

$$\lim_{M \rightarrow \infty} \frac{\rho_A(\mathbf{x})}{M} = \rho^{GP}(\mathbf{x}), \quad \lim_{M \rightarrow \infty} \frac{\rho_B(\mathbf{y})}{M} = \rho^{GP}(\mathbf{y}), \quad (45)$$

and

$$\lim_{M \rightarrow \infty} \frac{\rho_{AB}(\mathbf{x}, \mathbf{y})}{M^2} = \rho^{GP}(\mathbf{x}) \rho^{GP}(\mathbf{y}). \quad (46)$$

With (43), (45), and (46), we have proved and established that the many-body energy and densities of the mixture coincide with their mean-field values in the infinite-particle limit. This constitutes a generalization for mixtures of Bose-Einstein condensates, at least within the mixture's HIM model, of what is known in the literature for single-species trapped Bose-Einstein condensates [62, 63].

D. Center-of-mass variance and uncertainty product

So far we have discussed the energy and densities of the mixture, and have established the relations in the infinite-particle limit in which the exact solution and the Gross-Pitaevskii theory coincide. As has recently been shown for single-species Bose-Einstein condensates, the variance of many-particle operators can deviate strongly when the many-body and mean-field treatments are compared [66, 67]. These quantities have recently been found to be sensitive to correlations in single-species Bose-Einstein condensates even in the infinite-particle limit. The many-body and mean-field analytical solutions of the mixture allow us to examine directly the variances of the center-of-mass position and momentum operators of the mixture, as well as their uncertainty product. We shall keep the discussion concise.

Consider the center-of-mass position and momentum operators of the mixture

$$\begin{aligned} \hat{\mathbf{R}}_{CM} &= \frac{1}{N} \sum_{j=1}^M (\mathbf{x}_j + \mathbf{y}_j) = \frac{1}{\sqrt{N}} \mathbf{Q}_N, \quad \hat{\mathbf{P}}_{CM} = \sum_{j=1}^M \left(\frac{1}{i} \frac{\partial}{\partial \mathbf{x}_j} + \frac{1}{i} \frac{\partial}{\partial \mathbf{y}_j} \right) = \sqrt{N} \frac{1}{i} \frac{\partial}{\partial \mathbf{Q}_N}, \\ [\hat{\mathbf{R}}_{CM}, \hat{\mathbf{P}}_{CM}] &= \mathbf{i}, \quad \forall N, \end{aligned} \quad (47)$$

where \mathbf{i} (and analogously $\mathbf{1}$ below) is a shorthand symbol for i in each of the three Cartesian components. $\hat{\mathbf{R}}_{CM}$ and $\hat{\mathbf{P}}_{CM}$ are one-particle operators in the sense that they are linear with respect to all particles in the mixture. To compute their variances we need also the operators squares, $\hat{\mathbf{R}}_{CM}^2$ and $\hat{\mathbf{P}}_{CM}^2$, which are two-particle operators. These would lead to differences between the many-body and mean-field results; see for an extended discussion of the matter in the case of single-species Bose-Einstein condensates [66, 67].

We can now compute the variances of the center-of-mass position and momentum oper-

ators,

$$\begin{aligned}\Delta_{\hat{\mathbf{R}}_{CM}}^2 &= \langle \Psi | \hat{\mathbf{R}}_{CM}^2 | \Psi \rangle - \langle \Psi | \hat{\mathbf{R}}_{CM} | \Psi \rangle^2 = \frac{1}{N} \times \frac{1}{2\omega} \mathbf{1}, \\ \Delta_{\hat{\mathbf{P}}_{CM}}^2 &= \langle \Psi | \hat{\mathbf{P}}_{CM}^2 | \Psi \rangle - \langle \Psi | \hat{\mathbf{P}}_{CM} | \Psi \rangle^2 = N \times \frac{\omega}{2} \mathbf{1}, \quad \forall N,\end{aligned}\tag{48}$$

which are straightforwardly obtained due to the separability of the wave-function (9). For comparison, the corresponding expressions at the Gross-Pitaevskii level are computed from the mean-field wave-function (36) and given by

$$\begin{aligned}\Delta_{\hat{\mathbf{R}}_{CM,GP}}^2 &= \langle \Phi^{GP} | \hat{\mathbf{R}}_{CM}^2 | \Phi^{GP} \rangle - \langle \Phi^{GP} | \hat{\mathbf{R}}_{CM} | \Phi^{GP} \rangle^2 = \frac{1}{N} \times \frac{1}{2\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}} \mathbf{1}, \\ \Delta_{\hat{\mathbf{P}}_{CM,GP}}^2 &= \langle \Phi^{GP} | \hat{\mathbf{P}}_{CM}^2 | \Phi^{GP} \rangle - \langle \Phi^{GP} | \hat{\mathbf{P}}_{CM} | \Phi^{GP} \rangle^2 = N \times \frac{\sqrt{\omega^2 + 2(\Lambda_1 + \Lambda_2)}}{2} \mathbf{1}, \quad \forall N.\end{aligned}\tag{49}$$

Comparing (48) and (49) we see how the self-consistency of the Gross-Pitaevskii orbital (40), whose shape depends on the sum of the intra- and inter-species interaction parameters $\Lambda_1 + \Lambda_2$, alters the values of the mean-field variances in comparison with the exact result. This is an interesting result for the mixture which is best expressed by the respective ratios

$$\frac{\Delta_{\hat{\mathbf{R}}_{CM,GP}}^2}{\Delta_{\hat{\mathbf{R}}_{CM}}^2} = \frac{1}{\sqrt{1 + \frac{2}{\omega^2}(\Lambda_1 + \Lambda_2)}} \mathbf{1}, \quad \frac{\Delta_{\hat{\mathbf{P}}_{CM,GP}}^2}{\Delta_{\hat{\mathbf{P}}_{CM}}^2} = \sqrt{1 + \frac{2}{\omega^2}(\Lambda_1 + \Lambda_2)} \mathbf{1}, \quad \forall N,\tag{50}$$

in which the total number of particles does not appear. In particular for predominantly attractive mixtures, $\Lambda_1 + \Lambda_2 > 0$, since the sum $\Lambda_1 + \Lambda_2$ is unbound from above the ratio between the mean-field and exact center-of-mass position variances (50) can be as small as one wishes. However, the ratio of the center-of-mass momentum variances (50) is then, inevitably, very large.

We can now discuss the uncertainty product. Here, because the trap and all interactions are harmonic, the center-of-mass wave-function is a Gaussian and the mean-field orbital is a Gaussian as well, although being dressed by the particle-particle interactions. Consequently,

$$\Delta_{\hat{\mathbf{R}}_{CM}}^2 \Delta_{\hat{\mathbf{P}}_{CM}}^2 = \frac{1}{4} \mathbf{1}, \quad \Delta_{\hat{\mathbf{R}}_{CM,GP}}^2 \Delta_{\hat{\mathbf{P}}_{CM,GP}}^2 = \frac{1}{4} \mathbf{1}, \quad \forall N,\tag{51}$$

irrespective to the interactions between the particles. The comparison between the exact and mean-field solutions in terms of the uncertainty product might erroneously imply that there are no correlations in the mixture, especially in the limit of an infinite number of particles. Here, the correlations which survive the infinite-particle limit can for instance be

seen in the ratios of the variances (50). Although not discussed in [53], this generalizes the situation for the single-species HIM to the mixture's HIM model.

A final note. The result (51) raises the useful question what happens for general intra- and inter-species interactions. Is this equivalence between the center-of-mass uncertainty products at the exact and mean-field levels lifted? The answer goes beyond the solution of the HIM model for mixtures but, together with the related issue of an explicit construction of the center-of-mass separability in the generic case, is presented for completeness in the Appendix.

IV. CONCLUDING REMARKS

We have presented in this work a solvable quantum model for a mixture of two trapped Bose-Einstein condensates. The model consists of two kinds of identical bosons, A and B , held in a harmonic potential and interacting by harmonic particle-particle interactions, namely, the harmonic-interaction model for mixtures. We have concentrated in the present investigation on the case of a symmetric mixture in which the number of bosons and interactions within species A are the same as for species B . By generalizing the treatment of Cohen and Lee [53] to mixtures, closed form expressions for the ground-state energy, wave-function, and lowest-order intra- and inter-species densities are obtained. These quantities are analyzed analytically as a function of the number of particles and the intra- and inter-species interactions.

Aside from the many-body solution, we have also obtained analytically the Gross-Pitaevskii solution for the ground-state, as far as demixing of the two Bose-Einstein condensates is excluded. This has allowed us to compare the exact, many-body and mean-field solutions for any number of particles. In particular, keeping the products of the number of particles times the intra-species and inter-species interaction strengths fixed, while increasing the number of particles in the mixture, we were able to prove that the exact ground-state energy and lowest-order intra-species and inter-species densities converge at the infinite-particle limit to the results of the Gross-Pitaevskii theory for the mixture. This holds as a particular generalization for bosonic mixtures of the known literature results for single-species bosons [62, 63]. On the other end, the separability of the mixture's center-of-mass coordinate is used to show that the result for the variance of many-particle operators in

the mixture obtained within Gross-Pitaevskii theory for mixtures can deviate substantially from the exact, many-body result, even in the limit of an infinite number of particles. The present analytical results hence show that many-body correlations exist in the ground state of a trapped mixture of Bose-Einstein condensates made of any number of particles, thus generalizing our recent result for single-species bosons [66].

As an outlook we mention the asymmetric mixture, out-of-equilibrium dynamics, and more, all within the harmonic-interaction model for mixtures. In particular, an impurity made of one or two particles would be interesting to solve, once the techniques used above are adapted to asymmetric integrations. Last but not least, we hope that the present analytical results and proofs obtained in the limit of an infinite number of particles for a particular solvable model would stimulate generalizations for mixtures with short-range interactions, in as much as single-species bosons were offered mathematically rigorous results in this limit in the literature.

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Appendix A: Center-of-mass separability and uncertainty product for a mixture with generic particle-particle interactions

Let the Hamiltonian of the mixture with generic particle-particle interactions be

$$\begin{aligned} \hat{H}(\mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}_1, \dots, \mathbf{y}_M) = & \sum_{j=1}^M \left[\left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{x}_j^2} + \frac{1}{2} \omega^2 \mathbf{x}_j^2 \right) + \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{y}_j^2} + \frac{1}{2} \omega^2 \mathbf{y}_j^2 \right) \right] + \\ & + \lambda_1 \sum_{1 \leq j < k}^M [W_1(\mathbf{x}_j - \mathbf{x}_k) + W_1(\mathbf{y}_j - \mathbf{y}_k)] + \lambda_2 \sum_{j=1}^M \sum_{k=1}^M W_2(\mathbf{x}_j - \mathbf{y}_k). \end{aligned} \quad (\text{A1})$$

With the ansatz $\Phi^{GP}(\mathbf{x}_1, \dots, \mathbf{x}_M, \mathbf{y}_1, \dots, \mathbf{y}_M) = \prod_{j=1}^M \phi(\mathbf{x}_j) \prod_{k=1}^M \phi(\mathbf{y}_k)$ [Eq. (36)], i.e., when excluding demixing in the ground state, the mixture's Gross-Pitaevskii energy functional

reduces to

$$\begin{aligned} \varepsilon^{GP} = & \int d\mathbf{r} \phi^*(\mathbf{r}) \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{1}{2} \omega^2 \mathbf{r}^2 \right) \phi(\mathbf{r}) + \\ & + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' |\phi(\mathbf{r})|^2 |\phi(\mathbf{r}')|^2 [\Lambda_1 W_1(\mathbf{r} - \mathbf{r}') + \Lambda_2 W_2(\mathbf{r} - \mathbf{r}')], \end{aligned} \quad (\text{A2})$$

and the resulting Gross-Pitaevskii equations degenerate to one

$$\left\{ -\frac{1}{2} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{1}{2} \omega^2 \mathbf{r}^2 + \int d\mathbf{r}' |\phi(\mathbf{r}')|^2 [\Lambda_1 W_1(\mathbf{r} - \mathbf{r}') + \Lambda_2 W_2(\mathbf{r} - \mathbf{r}')] \right\} \phi(\mathbf{r}) = \mu \phi(\mathbf{r}). \quad (\text{A3})$$

The generic intra-species W_1 and inter-species W_2 interactions are seen to dress the Gross-Pitaevskii orbital ϕ of the A and B species in the mixture to a shape different than the Gaussian in (40). The reason is that the mean-field potential $\int d\mathbf{r}' |\phi(\mathbf{r}')|^2 [\Lambda_1 W_1(\mathbf{r} - \mathbf{r}') + \Lambda_2 W_2(\mathbf{r} - \mathbf{r}')]$ for generic interactions is different than \mathbf{r}^2 .

Next, we comment on the separability of the center-of-mass coordinate \mathbf{Q}_N in the ground state of the Hamiltonian (A1), namely, we show that the coordinates needed to express the interaction terms are all but \mathbf{Q}_N . This has been shown explicitly in the main text by diagonalizing the interaction terms of the mixture's HIM, but such diagonalizing cannot be made with generic particle-particle interactions.

This is clearly the case for the intra-species interaction terms $W_1(\mathbf{x}_j - \mathbf{x}_k)$ and $W_1(\mathbf{y}_j - \mathbf{y}_k)$ on the account of the relative coordinates $\mathbf{Q}_1, \dots, \mathbf{Q}_{M-1}$ and $\mathbf{Q}_M, \dots, \mathbf{Q}_{2(M-1)}$ of each species separately, see (3). But what about the inter-species interaction terms $W_2(\mathbf{x}_j - \mathbf{y}_k)$? To express them, adding \mathbf{Q}_{N-1} , the relative coordinate between the center-of-mass of the A and the center-of-mass of the B species, suffices. To illustrate this point, consider the inter-species relative coordinate $\mathbf{x}_M - \mathbf{y}_M$ which can be expressed as follows:

$$\mathbf{x}_M - \mathbf{y}_M = \sqrt{\frac{M-1}{M}} [\mathbf{Q}_{M-1} - \mathbf{Q}_{2(M-1)}] + \sqrt{\frac{2}{M}} \mathbf{Q}_{N-1}. \quad (\text{A4})$$

The other inter-species relative coordinate $\mathbf{x}_j - \mathbf{y}_k$ can be expressed analogously, using the fact that the relative coordinates of each species separately, $\mathbf{Q}_1, \dots, \mathbf{Q}_{M-1}$ and $\mathbf{Q}_M, \dots, \mathbf{Q}_{2(M-1)}$, can be intermixed at will to generate any of the permutations of \mathbf{Q}_{M-1} and of $\mathbf{Q}_{2(M-1)}$ with respect to the $\mathbf{x}_1, \dots, \mathbf{x}_M$ and $\mathbf{y}_1, \dots, \mathbf{y}_M$ coordinates, respectively.

All in all, the Hamiltonian (A1) is separable in the sense that $\hat{H} = \left(-\frac{1}{2} \frac{\partial^2}{\partial \mathbf{Q}^2} + \frac{1}{2} \omega^2 \mathbf{Q}_N^2 \right) + \hat{H}_{rel}(\mathbf{Q}_1, \dots, \mathbf{Q}_{N-1})$, and so does its ground state, $\Psi = \left(\frac{\omega}{\pi} \right)^{\frac{3}{4}} e^{-\frac{1}{2} \omega \mathbf{Q}_N^2} \Psi_{rel}(\mathbf{Q}_1, \dots, \mathbf{Q}_{N-1})$. Here ‘rel’ stands for all but center-of-mass quantities. Consequently, for mixtures with

generic particle-particle interactions W_1 and W_2 the uncertainty products computed at the many-body and mean-field levels, not just the individual center-of-mass position and momentum quantities, like the ratios (50) discussed above, differ from each other even in the infinite-particle limit. Put in formulas,

$$\Delta_{\mathbf{R}_{CM},GP}^2 \Delta_{\mathbf{P}_{CM},GP}^2 > \Delta_{\mathbf{R}_{CM}}^2 \Delta_{\mathbf{P}_{CM}}^2 = \frac{1}{4} \mathbf{1}, \quad \forall N, \quad (\text{A5})$$

which concludes our discussion.

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